1,5-Dimethyl-6-phenyl-1,6-dihydro-3-pyridinecarbonitrile

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.95	0.69	0.95	0.65	0.96	0.68

Model Results

Predicted value: 7.45

Global applicability domain: Inside

Local applicability domain index: 9.86e-01

Confidence level: 8.78e-01

Nearest Neighbors from the Training Set

Image not found

1,3,5-Trichloronaphthalene
Measured: 7.32
Predicted: 7.45

Image not found

Phenanthrene
Measured: 7.57
Predicted: 7.50

Image not found

Anthracene
Measured: 7.55
Predicted: 7.50